Shot noise in electron transport through a double quantum dot: a master equation approach*

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We study shot noise in tunneling current through a double quantum dot connected to two electric leads. We derive two master equations in the occupation-state basis and the eigenstate basis to describe the electron dynamics. The approach based on the occupation-state basis, despite being widely used in many previous studies, is valid only when the interdot coupling strength is much smaller than the energy difference between the two dots. In contrast, the calculations using the eigenstate basis are valid for an arbitrary interdot coupling. Using realistic model parameters, we demonstrate that the predicted currents and shot-noise properties from the two approaches are significantly different when the interdot coupling is not small. Furthermore, properties of the shot noise predicted using the eigenstate basis successfully reproduce qualitative features found in a recent experiment.

Keywords: double quantum dot, master equation approach, shot noise in tunneling current

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1. Introduction

The precise control of coherent coupling between quantum states is of great importance in quantum information processing. Recent studies show that artificial two-level systems designed using mesoscopic circuits can be controlled in nanosecond time scales and can also exhibit coherent oscillations between two quantum states (see, e.g., Refs. [1]–[3]). A double quantum dot (DQD) provides a useful system to explore coherent effects because interdot hopping intrinsically couples states in two different dots and is tunable via the gate voltage.[4,5] A commonly used observable for studying the effects of coherent coupling is the current through the DQD.[6] Recently, shot-noise measurement has been demonstrated as another useful tool for studying the coherent effects.[7,8] Moreover, the shot-noise properties have been predicted to be an indicator of the degree of entanglement between electron states[9,10] and they are also related to the radiative decay properties of the one-demensional quantum ring exciton.[11]

Shot noise, i.e., current fluctuations due to the discrete and stochastic nature of electron transport, describes the correlation between electrons transported successively through mesoscopic systems, such as quantum dots (QDs) or molecular devices (for reviews, see Refs. [12] and [13]). In classical transport, the noise is typically Poissonian with a power density $S = 2e\langle I\rangle$, where e is the unit charge and $\langle I\rangle$ is the average current. However, either Coulomb interaction or the Pauli's exclusion principle can induce a negative correlation between successive transport events. This reduces the noise power density so that $S < 2e\langle I\rangle$ corresponding to a sub-Poissonian noise.[14] In contrast, the interplay between Coulomb interaction and the Pauli's exclusion principle can also produce a positive correlation between the transport events, i.e., $S > 2e\langle I\rangle$. This corresponds to a super-Poissonian noise. The Fano factor $F = S/2e\langle I\rangle$ is usually used to characterize the shot noise, where $F = 1$, $F > 1$, or $F < 1$, respectively, corresponds to the Poissonian, super-Poissonian, or sub-Poissonian noise. Many theoretical works show that super-Poissonian noise of electron,[15–17] or spin,[18–21] and positive cross correlation between different spin states[22] in QDs can be

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induced via dynamical channel blockade. Moreover, a super-Poissonian noise in tunneling current caused by dynamical channel blockade has been observed in a system consisting of two electrostatically coupled QDs[23] and also a single QD[24,25] in recent experiments.

In this work, we study the current and shot-noise in electrons tunneling through a DQD. We employ two different approaches and compare the results. First, we follow many previous investigations (see, e.g., Refs. [8] and [26]–[29]) and derive a master equation for the electron transport in the occupation-state basis of the DQD. We show that to arrive at this master equation, one needs to assume that the interdot coupling strength is much smaller than the energy difference between the two dots. Alternatively, we derive a more generally applicable master equation in the eigenstate basis of the DQD, which does not require the assumption of a small interdot coupling and is hence valid for any arbitrary interdot coupling strength. Similar eigenstate basis was used in non-equilibrium Green function approaches to study current–voltage asymmetry,[30] inelastic transport,[31] and transport phenomenon related to the on-site Coulomb interaction of electrons in QDs.[32] Also, master equations in the eigenstate basis was used to study the transport properties of QDs related to the effects of Pauli spin blockade[33] and electron cotunneling process.[34,35] Here the two master equations (i.e., the master equation in the occupation-state basis and that in the eigenstate basis) are formally different in general and are identical only in the limiting case when the interdot coupling is much smaller than the energy difference between the two dots. We show that for small interdot coupling, the properties of the shot noise predicted by the two master equations agree with each other as expected. However, for large interdot coupling, they are significantly different.

The present paper is organised as follows. In Section 2, we introduce the model for a DQD connected to two electric leads. A phonon bath that affects the dynamics of the DQD is also considered. Two master equations for the electron dynamics in the DQD are derived in both the occupation-state basis and the eigenstate basis. In Sections 3 and 4, we study, respectively, the properties of the current through the DQD and the associated shot noise. Results based on the two master equations are compared. Moreover, a brief conclusion is presented in Section 5.

2. Time evolution of the reduced density matrix of a double quantum dot

The schematic diagram of a DQD connected to two electrodes by tunneling barriers is shown in Fig. 1. The voltage across the DQD is biased so that the chemical potential of the left electrode $\mu_{\rm L}$ is higher than that of the right electrode $\mu_{\rm R}$. Thus, an electron can tunnel from the left electrode to the right one via the DQD. We assume that the DQD is in the Coulomb regime (with both strong intra- and interdot Coulomb repulsions), so that at most a single electron is allowed in the DQD. In the occupation representation, the electron basis states are the vacuum state $|0\rangle$, the state with one electron in the left dot $|1\rangle$, and the state with one electron in the right dot $|2\rangle$.

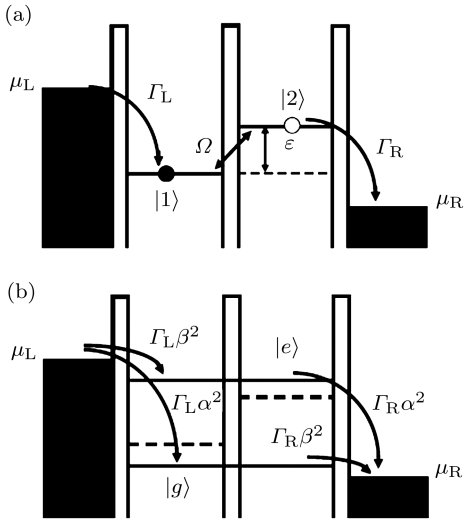


Fig. 1. Schematic diagram of an electron transported through a DQD connected to two electric leads via tunneling barriers. (a) Considering DQD electron states in the occupation-state basis, the electron tunnels sequentially from the left lead to the right lead via first the left dot and then the right dot. (b) Considering the eigenstate basis, the electron is transported via either the ground-state channel or the excited-state channel. The effective tunneling rates from the left lead to the ground state and the excited state are $\Gamma_{\rm L}\alpha^2$ and $\Gamma_{\rm L}\beta^2$, while those from the ground state and the excited state to the right lead are $\Gamma_{\rm R}\beta^2$ and $\Gamma_{\rm R}\alpha^2$.

The Hamiltonian of the whole system reads (taking $\hbar = 1$)

$$H_{\rm tot} = H_{\rm leads} + H_{\rm DQD} + H_{\rm T} + H_{\rm ph} + H_{\rm ep}. \quad (1)$$

The first two terms $H_{\rm leads}$ and $H_{\rm DQD}$ are respectively the Hamiltonians of the two electrodes and the DQD,

which are given by

$$H_{\rm leads} = \sum_{\alpha k} \omega_{\alpha k} c^{+}_{\alpha k} c_{\alpha k}, \tag{2}$$

$$H_{\rm DQD} = \frac{\varepsilon}{2}\sigma_z + \Omega\sigma_x, \tag{3}$$

where $c^{+}_{\alpha k}(c_{\alpha k})$ is the creation (annihilation) operator of an electron with momentum k in the electrode $\alpha(\alpha = {\rm l}, {\rm r})$; $\sigma_z = a^{+}_2 a_2 - a^{+}_1 a_1$ and $\sigma_x = a^{+}_2 a_1 + a^{+}_1 a_2$ are the Pauli matrices, with $a^{+}_1(a^{+}_2)$ being the electron creation operator in the left (right) dot of the DQD. In Eq. (3), the first term $\varepsilon\sigma_z/2$, with $\varepsilon = \varepsilon_2 - \varepsilon_1$ denoting the energy difference between the two dots, gives the Hamiltonian of the two uncoupled quantum dots, while the second term $\Omega\sigma_x$ characterises the interdot hopping. The tunneling coupling between the DQD and the electrodes is described by

$$H_{\rm T} = \sum_{k} \left(\Omega_{{\rm l}k} a^{+}_1 c_{{\rm l}k} + \Omega_{{\rm r}k} a^{+}_2 \Upsilon_{\rm r} c_{{\rm r}k} + {\rm H.c.}\right), \tag{4}$$

where $\Omega_{{\rm l}k({\rm r}k)}$ is the tunneling strength between the QD and the left (right) electrode. The operators $\Upsilon_{\rm r}(\Upsilon^{+}_{\rm r})$ decreases (increases) the number of electrons having tunneled into the right lead (via the barrier between the DQD and the right lead).[36] These counting operators allow one to keep track of the tunneling process during the evolution of the DQD. Below we focus on current and shot noise in electron tunneling through the right tunneling barrier, so only the related counting operators ($\Upsilon_{\rm r}$ and $\Upsilon^{+}_{\rm r}$) are introduced in the tunneling Hamiltonian (4).

Also, we consider the effects of the phonon-bath environment on the evolution of the DQD. The Hamiltonian of this phonon bath is

$$H_{\rm ph} = \sum_{q} \omega_q b^{+}_q b_q \tag{5}$$

with $b^{+}_q(b_q)$ creating (annihilating) a phonon with frequency ω_q. The electron–phonon interaction is given by

$$H_{\rm ep} = \sigma_x \sum_{q} \lambda_q \left(b^{+}_q + b_q\right), \tag{6}$$

where λ_q is the electron–phonon coupling strength.

The evolution of the whole system is described by the von Neumann equation for the density matrix $\boldsymbol{\rho}_{\rm R}$ of the whole system

$$\dot{\boldsymbol{\rho}}_{\rm R}(t) = -{\rm i}\left[H_{\rm tot}, \boldsymbol{\rho}_{\rm R}(t)\right]. \tag{7}$$

Here we are interested in the time evolution of the DQD and treat both the electric leads and the phonon bath as the total outside environment. We will hence derive the master equation of the reduced density matrix $\boldsymbol{\rho}_{\rm d}(t)$ of the DQD: $\boldsymbol{\rho}_{\rm d}(t) = {\rm Tr}_{\rm E}\{\boldsymbol{\rho}_{\rm R}(t)\}$, where ${\rm Tr}_{\rm E}\{\cdots\}$ denotes the trace over the degrees of freedom of both the electric leads and the phonon bath. In our calculation, we adopt the interaction picture based on the free Hamiltonian

$$H_0 = H_{\rm leads} + H_{\rm DQD} + H_{\rm ph}, \tag{8}$$

and the interaction Hamiltonian becomes

$$H_{\rm int}(t) = H_{\rm T}(t) + H_{\rm ep}(t), \tag{9}$$

where operators in the interaction and the Schrödinger pictures are related by $A(t) = {\rm e}^{{\rm i}H_0 t} A\, {\rm e}^{-{\rm i}H_0 t}$ for any operator A.

After tracing over the degrees of freedom of both the electrodes and the phonon bath, one obtains the master equation for the reduced density matrix $\boldsymbol{\rho}^{\rm I}_{\rm d}$ of the DQD in the interaction picture as[37]

$$\begin{aligned}&\dot{\boldsymbol{\rho}}^{\rm I}_{\rm d}(t)\\ &= -{\rm i}{\rm Tr}_{\rm E}\left[H_{\rm int}(t), \boldsymbol{\rho}_{\rm d}(0)\boldsymbol{\rho}_{\rm E}(0)\right] - {\rm Tr}_{\rm E}\int_0^t {\rm d}t'\\ &\quad\left[H_{\rm int}(t), \left[H_{\rm int}(t'), \boldsymbol{\rho}^{\rm I}_{\rm d}(t')\otimes\boldsymbol{\rho}_{\rm E}(0)\right]\right],\end{aligned} \tag{10}$$

where $\boldsymbol{\rho}_{\rm E}$ is the density matrix of the outside environment. Because the trace of a single unpaired creation or annihilation operator over the lead or the phonon bath is zero, e.g., ${\rm Tr}_{\rm E}\{c_{lk}\boldsymbol{\rho}_E\} = 0$, the first term in Eq. (10) vanishes. Substituting the interaction term Eq. (9) into Eq. (10), within the Born–Markov approximation, one can obtain

$$\dot{\boldsymbol{\rho}}^{\rm I}_{\rm d}(t) = L_{\rm T}\boldsymbol{\rho}^{\rm I}_{\rm d}(t) + L_{\rm ph}\rho^{\rm I}_{\rm d}(t). \tag{11}$$

Here, the dissipative part due to the electric leads is given by

$$\begin{aligned}&L_{\rm T}\boldsymbol{\rho}^{\rm I}_{\rm d}(t)\\ &= -\sum_{\alpha={\rm l,r}} {\rm Tr}_\alpha \int_0^t {\rm d}t'[H_{\rm T}(t)H_{\rm T}(t')\boldsymbol{\rho}^{\rm I}_{\rm d}(t)\boldsymbol{\rho}_{\rm leads}\\ &\quad - H_{\rm T}(t)\rho^{\rm I}_{\rm d}(t)\boldsymbol{\rho}_{\rm leads}H_{\rm T}(t') + {\rm H.c.}],\end{aligned} \tag{12}$$

where $\boldsymbol{\rho}_{\rm leads}(0) = \boldsymbol{\rho}_{\rm L}(0)\otimes\boldsymbol{\rho}_{\rm R}(0)$ is the density matrix of the two electric leads. The dissipative part caused by the phonon bath is

$$\begin{aligned}L_{\rm ph}\boldsymbol{\rho}^{\rm I}_{\rm d}(t) = &-{\rm Tr}_{\rm ph}\int_0^t {\rm d}t'[H_{\rm ep}(t)H_{\rm ep}(t')\boldsymbol{\rho}^{\rm I}_{\rm d}(t)\rho_{\rm ph}\\ &-H_{\rm ep}(t)\rho^{\rm I}_{\rm d}(t)\rho_{\rm ph}H_{\rm ep}(t') + {\rm H.c.}].\end{aligned} \tag{13}$$

From Eqs. (11)–(13), one can derive the master equation for the n-resolved reduced density matrix $\boldsymbol{\rho}_{\rm d}^{(n)}(t)$ of the DQD, where $\boldsymbol{\rho}_{\rm d}^{(n)}(t) = \langle n|\,\boldsymbol{\rho}_{\rm d}(t)\,|n\rangle$ and n is the number of electrons that have arrived at the right lead at time t.

2.1. Master equation in the occupation-state basis

The master equation of the DQD in the occupation-state basis was previously used to study the current properties[26−29] and shot-noise properties[8,17,20,21] of electrons tunneling through the DQD. In the interaction picture defined by the free Hamiltonian H_0 in Eq. (8), the unperturbed evolution operator $U_0(t) = {\rm e}^{{\rm i}H_0 t}$ is difficult to calculate in the occupation-state basis in the presence of interdot coupling. One hence splits H_0 into two parts

$$H_0 = H_1 + H_\Omega, \tag{14}$$

where

$$H_1 = H_{\rm leads} + H_{\rm ph} + \frac{\varepsilon}{2}\sigma_z, \tag{15}$$

$$H_\Omega = \Omega\sigma_x. \tag{16}$$

Following previously works[37,38] on deriving master equations in the occupation-state basis, we assume that the interdot couping Ω is small and satisfies $\Omega \ll |\varepsilon_2 - \varepsilon_1|$, thus we have $H_0 \approx H_1$. The evolution operator can then be approximated as

$${\rm e}^{{\rm i}H_0 t} \approx {\rm e}^{{\rm i}H_1 t}. \tag{17}$$

With this approximation, one easily obtains

$$\begin{aligned} H_{\rm T}(t) \approx \sum_k [&\Omega_{{\rm l}k} a_1^+ c_{{\rm l}k}\,{\rm e}^{-{\rm i}(\omega_{{\rm l}k}-\omega_1)t} \\ &+\Omega_{{\rm r}k}\Upsilon_{\rm r} a_2^+ c_{{\rm r}k}\,{\rm e}^{-{\rm i}(\omega_{{\rm r}k}-\omega_2)t} + {\rm H.c.}], \end{aligned} \tag{18}$$

and

$$\begin{aligned} H_{\rm ep}(t) \approx &\left(\sigma_+\,{\rm e}^{{\rm i}\varepsilon t} + \sigma_-\,{\rm e}^{-{\rm i}\varepsilon t}\right) \\ &\times \sum_q \lambda_q \left(b_q^+\,{\rm e}^{{\rm i}\omega_q t} + b_q\,{\rm e}^{-{\rm i}\omega_q t}\right), \end{aligned} \tag{19}$$

where $\omega_{1,2} = \mp\varepsilon/2$. Here $\sigma_+ = a_2^+ a_1$ and $\sigma_- = a_1^+ a_2$ are the raising and lowering operators in the occupation-state basis.

We consider the nonequilibrium case with a large bias voltage across the DQD, so that all energy levels of the DQD lie within the bias window, as shown in Figs. 1(a) and 1(b). Substituting Eqs. (18) and (19) into Eqs. (11)–(13), taking the trace over the degrees of freedom of both the two electrodes and the phonon bath, and converting the obtained equation to the Schrödinger picture, one arrives at the master equation in the occupation-state basis for a weak interdot coupling $\Omega \ll |\varepsilon_2 - \varepsilon_1|$,[37]

$$\begin{aligned} \dot{\boldsymbol{\rho}}_{\rm d}(t) = &-{\rm i}\left[H_{\rm DQD}, \boldsymbol{\rho}_{\rm d}(t)\right] + \frac{\Gamma_{\rm L}}{2} D\left[a_1^+\right]\boldsymbol{\rho}_{\rm d}(t) \\ &+\frac{\Gamma_{\rm R}}{2} D\left[\Upsilon_{\rm r}^+ a_2\right]\boldsymbol{\rho}_{\rm d}(t) + \frac{\gamma_1}{2} D\left[\sigma_-\right]\boldsymbol{\rho}_{\rm d}(t) \\ &+\frac{\gamma_2}{2} D\left[\sigma_+\right]\boldsymbol{\rho}_{\rm d}(t), \end{aligned} \tag{20}$$

where $\Gamma_{\rm L(R)} = 2\pi\rho_{{\rm l}k({\rm r}k)}\Omega_{{\rm l}k({\rm r}k)}^2$ is the electron tunneling rate through the left (right) tunneling barrier. Here, the electron density of states $\rho_{\alpha k}$ at lead $\alpha(\alpha = {\rm l}, {\rm r})$ and the tunneling strength $\Omega_{\alpha k}$ are assumed to be energy-independent. The notation D acting on any operator A is defined as

$$D[A]\boldsymbol{\rho} = 2A\boldsymbol{\rho}A^+ - \left[A^+A\boldsymbol{\rho} + \boldsymbol{\rho}A^+A\right]. \tag{21}$$

The dissipation rates induced by the electron–phonon interaction are

$$\begin{aligned} \gamma_{1,2} = &\,2\pi\left\{J(\pm\varepsilon)\left[n(\pm\varepsilon)+1\right]\right. \\ &\left.+\,J(\mp\varepsilon)\,n(\mp\varepsilon)\right\}, \end{aligned} \tag{22}$$

where $J(\omega) = \sum_q \lambda_q^2\delta(\omega-\omega_q)$ is the bath spectral density, and $n(\omega) = \left[\exp(\omega/k_{\rm B}T)-1\right]^{-1}$ is the average phonon number at temperature T. Using Eq. (20) and the following relations[36]

$$\begin{aligned} &\langle n|\,\Upsilon_{\rm r}^+\Upsilon_{\rm r}\boldsymbol{\rho}_{\rm d}\,|n\rangle = \boldsymbol{\rho}_{\rm d}^{(n)}, \\ &\langle n|\,\Upsilon_{\rm r}\Upsilon_{\rm r}^+\boldsymbol{\rho}_{\rm d}\,|n\rangle = \boldsymbol{\rho}_{\rm d}^{(n)}, \\ &\langle n|\,\Upsilon_{\rm r}^+\boldsymbol{\rho}_{\rm d}\Upsilon_{\rm r}\,|n\rangle = \boldsymbol{\rho}_{\rm d}^{(n-1)}, \\ &\langle n|\,\Upsilon_{\rm r}\boldsymbol{\rho}_{\rm d}\Upsilon_{\rm r}^+\,|n\rangle = \boldsymbol{\rho}_{\rm d}^{(n+1)}, \end{aligned} \tag{23}$$

one obtains the equation of motion for each density matrix element

$$\begin{aligned} \dot{\rho}_{00}^{(n)}(t) &= -\Gamma_{\rm L}\rho_{00}^{(n)} + \Gamma_{\rm R}\rho_{22}^{(n-1)}, \\ \dot{\rho}_{11}^{(n)}(t) &= \Gamma_{\rm L}\rho_{00}^{(n)} + {\rm i}\Omega\left(\rho_{12}^{(n)} - \rho_{21}^{(n)}\right) \\ &\quad + \gamma_1\rho_{22}^{(n)} - \gamma_2\rho_{11}^{(n)}, \\ \dot{\rho}_{22}^{(n)}(t) &= -\Gamma_{\rm R}\rho_{22}^{(n)} - {\rm i}\Omega\left(\rho_{12}^{(n)} - \rho_{21}^{(n)}\right) \\ &\quad - \gamma_1\rho_{22}^{(n)} + \gamma_2\rho_{11}^{(n)}, \\ \dot{\rho}_{12}^{(n)}(t) &= {\rm i}\varepsilon\rho_{12}^{(n)} + {\rm i}\Omega\left(\rho_{11}^{(n)} - \rho_{22}^{(n)}\right) \\ &\quad - \frac{\Gamma_{\rm R} + \gamma_1 + \gamma_2}{2}\rho_{12}^{(n)}. \end{aligned} \tag{24}$$

Then, the ith diagonal matrix element $\rho_{ii} = \sum_n \rho_{ii}^{(n)}$ ($i = 0$, 1, or 2) gives the occupation probability of the state $|i\rangle$. The off-diagonal matrix element $\rho_{12}(t) = \sum_n \rho_{12}^{(n)}$ describes the coherence between states $|1\rangle$ and $|2\rangle$, and $\rho_{12}(t) = \rho_{21}^{*}(t)$. This master equation was used in many previous studies, e.g., Refs. [26] and [27].

The physical meaning of the master equation can be understood as follows. Take the equation for $\rho_{11}^{(n)}$ in Eq. (24) for example. The first term on the right-hand side describes the process of an electron tunneling from the left lead to the left dot with rate $\Gamma_{\rm L}$. The second term represents the coherent coupling between states $|1\rangle$ and $|2\rangle$ due to the interdot coupling. The third term describes the phonon-induced relaxation process from state $|2\rangle$ to $|1\rangle$ with rate γ_1. Finally, the fourth term describes the inverse process with rate γ_2.

2.2. Master equation in the eigenstate basis

As explained above, the master equation in the occupation-state basis is only valid for a weak interdot coupling. To extend the results to an arbitrary interdot coupling Ω, we now derive the master equation in the eigenstate basis of the DQD. The result is valid for any arbitrary interdot coupling strength.

Diagonalizing the Hamiltonian of the DQD [Eq. (3)], one has

$$H_{\rm DQD} = \frac{\Omega_0}{2}\left(|e\rangle\langle e| - |g\rangle\langle g|\right) = \frac{\Omega_0}{2}\sigma_z^{(e)}, \tag{25}$$

where $\Omega_0 = \sqrt{\varepsilon^2 + 4\Omega^2}$ is the energy splitting of the two eigenstates of the DQD given by

$$|g\rangle = \alpha|1\rangle - \beta|2\rangle\,, \quad |e\rangle = \beta|1\rangle + \alpha|2\rangle \tag{26}$$

with $\alpha \equiv \cos(\theta/2) = \sqrt{(\Omega_0+\varepsilon)/2\Omega_0}$, $\beta \equiv \sin(\theta/2) = \sqrt{(\Omega_0-\varepsilon)/2\Omega_0}$, and $\tan\theta = 2\Omega/\varepsilon$. The eigenstates and the occupation states are related by

$$|1\rangle = \alpha|g\rangle + \beta|e\rangle\,, \quad |2\rangle = -\beta|g\rangle + \alpha|e\rangle\,. \tag{27}$$

In the interaction picture based on the free Hamiltonian H_0 given by Eq. (8), the tunneling Hamiltonian [Eq. (4)] and the electron–phonon interaction [Eq. (6)], in the eigenstate basis, are given by

$$\begin{aligned} H_{\rm T}(t) &= \sum_k \Omega_{{\rm l}k}\left(\alpha a_{\rm g}^{+}\,{\rm e}^{{\rm i}\omega_{\rm g}t} + \beta a_{\rm e}^{+}\,{\rm e}^{{\rm i}\omega_{\rm e}t}\right)c_{{\rm l}k}\,{\rm e}^{-{\rm i}\omega_{{\rm l}k}t}] + \Omega_{{\rm r}k}\left(-\beta a_{\rm g}^{+}\,{\rm e}^{{\rm i}\omega_{\rm g}t} + \alpha a_{\rm e}^{+}\,{\rm e}^{{\rm i}\omega_{\rm e}t}\right)\Upsilon_{\rm r}c_{{\rm r}k}\,{\rm e}^{-{\rm i}\omega_{{\rm r}k}t} + {\rm H.c.},\\ H_{\rm ep} &= \left[\sigma_z^{(e)}\sin\theta + \cos\theta\left(\sigma_+^{(e)}\,{\rm e}^{{\rm i}\Omega_0 t} + \sigma_-^{(e)}\,{\rm e}^{-{\rm i}\Omega_0 t}\right)\right]\sum_q \lambda_q\left(b_q^{+}\,{\rm e}^{{\rm i}\omega_q t} + b_q\,{\rm e}^{-{\rm i}\omega_q t}\right), \end{aligned} \tag{28}$$

where $\omega_{g,e} = \mp\Omega_0/2$. Here $\sigma_+^{(e)} = a_{\rm e}^{+}a_{\rm g}$ and $\sigma_-^{(e)} = a_{\rm g}^{+}a_{\rm e}$ are the lowering and raising operators in the eigenstate basis.

Now, one can evaluate Eqs. (11)–(13) using Eq. (28). In the nonequilibrium case with a large bias voltage across the DQD, after converting the result to the Schrödinger picture, one obtains the master equation in the eigenstate basis which holds for any arbitrary interdot coupling Ω,[37]

$$\begin{aligned} \dot{\boldsymbol{\rho}}_{\rm d}(t) =& -{\rm i}\left[H_{\rm DQD}, \boldsymbol{\rho}_{\rm d}(t)\right] + \frac{\Gamma_{\rm L}}{2}\alpha^2 D\left[a_{\rm g}^{+}\right]\boldsymbol{\rho}_{\rm d} + \frac{\Gamma_{\rm L}}{2}\beta^2 D\left[a_{\rm e}^{+}\right]\boldsymbol{\rho}_{\rm d}\\ &+ \frac{\Gamma_{\rm R}}{2}\beta^2 D\left[a_{\rm g}\Upsilon_{\rm r}^{+}\right]\boldsymbol{\rho}_{\rm d} + \frac{\Gamma_{\rm R}}{2}\alpha^2 D\left[a_{\rm e}\Upsilon_{\rm r}^{+}\right]\boldsymbol{\rho}_{\rm d} + \frac{\lambda_1}{2}D\left[\sigma_-^{(e)}\right]\boldsymbol{\rho}_{\rm d} + \frac{\lambda_2}{2}D\left[\sigma_+^{(e)}\right]\boldsymbol{\rho}_{\rm d}, \end{aligned} \tag{29}$$

where

$$\begin{aligned} \lambda_1 &= 2\pi J(\Omega_0)\cos^2\theta\left[n(\Omega_0)+1\right],\\ \lambda_2 &= 2\pi J(\Omega_0)\cos^2\theta n(\Omega_0). \end{aligned} \tag{30}$$

Using Eq. (29), the n-resolved equation of motion for each density matrix element can be written as

$$\begin{aligned} \dot{\rho}_{00}^{(n)}(t) &= -\Gamma_{\rm L}\rho_{00}^{(n)} + \Gamma_{\rm R}\beta^2\rho_{gg}^{(n-1)} + \Gamma_{\rm R}\alpha^2\rho_{ee}^{(n-1)},\\ \dot{\rho}_{gg}^{(n)}(t) &= \Gamma_{\rm L}\alpha^2\rho_{00}^{(n)} - \Gamma_{\rm R}\beta^2\rho_{gg}^{(n)} + \lambda_1\rho_{ee}^{(n)} - \lambda_2\rho_{gg}^{(n)},\\ \dot{\rho}_{ee}^{(n)}(t) &= \Gamma_{\rm L}\beta^2\rho_{00}^{(n)} - \Gamma_{\rm R}\alpha^2\rho_{ee}^{(n)} - \lambda_1\rho_{ee}^{(n)} + \lambda_2\rho_{gg}^{(n)},\\ \dot{\rho}_{ge}^{(n)}(t) &= {\rm i}\Omega_0\rho_{ge}^{(n)} - \frac{\Gamma_0}{2}\rho_{ge}^{(n)}, \end{aligned} \tag{31}$$

where $\Gamma_0 = \Gamma_{\rm R} + \lambda_1 + \lambda_2$. It follows from Eq. (31) that the effective tunneling rate from the left lead to the ground (excited) state $|g\rangle$ ($|e\rangle$) is $\Gamma_{\rm L}\alpha^2$ ($\Gamma_{\rm L}\beta^2$), while the effective tunneling rate from the ground (excited)

state to the right lead is $\Gamma_{\rm R}\beta^2$ ($\Gamma_{\rm R}\alpha^2$) [see Fig. 1(b)]. We emphasise that these results derived in the eigenstate basis are valid for any arbitrary interdot coupling.

3. Current through the double quantum dot

To compare the master equations in Eqs. (24) and (31) derived, respectively, in the occupation-state basis and the eigenstate basis, we first apply them to study the tunneling current through the DQD. In the next section, the associated shot noise will also be studied. The current $I(t)$ through the DQD at time t is given by

$$I(t) = e\frac{{\rm d}N(t)}{{\rm d}t} = e\sum_{n,i} n\dot{\rho}_{ii}^{(n)}(t), \tag{32}$$

where $N(t)$ is the number of electrons that have tunneled into the right lead. Here, i is summed over all basis states of the basis used, i.e. $i = 0, 1, 2$ in the occupation-state basis and $i = 0, g, e$ in the eigenstate basis. Denoting results based on the occupation-state basis and the eigenstate basis by 'o' and 'e', values of the current $I_{\rm o}(t)$ and $I_{\rm e}(t)$ calculated using Eqs. (24) and (31) are respectively

$$I_{\rm o}(t) = e\Gamma_{\rm R}\rho_{22}(t), \tag{33a}$$

$$I_{\rm e}(t) = e\left[\Gamma_{\rm R}\beta^2\rho_{gg}(t) + \Gamma_{\rm R}\alpha^2\rho_{ee}(t)\right]. \tag{33b}$$

At steady-state with $\dot{\rho}_{ij}(t) = 0$ ($i, j = 0, 1, 2$ or $0, g, e$) the calculated values $I_{\rm o}^{\rm s}$ and $I_{\rm e}^{\rm s}$ of the stationary current are

$$I_{\rm o}^{\rm s} = \frac{e\Gamma_{\rm L}\Gamma_{\rm R}}{\Lambda}\Big\{\gamma_2\left[4\varepsilon^2 + (\gamma_1+\gamma_2+\Gamma_{\rm R})^2\right] + 4\Omega^2(\gamma_1+\gamma_2+\Gamma_{\rm R})\Big\}, \tag{34a}$$

$$I_{\rm e}^{\rm s} = \frac{e\Gamma_{\rm L}\Gamma_{\rm R}\left[\beta^2\lambda_1 + \alpha^2\left(\lambda_2 + \beta^2\Gamma_{\rm R}\right)\right]}{\Xi}, \tag{34b}$$

where

$$\begin{aligned}\Lambda = {} & 4\Omega^2\Gamma_{\rm R}(2\Gamma_{\rm L}+\Gamma_{\rm R}) + (\gamma_2+\Gamma_{\rm L})\Gamma_{\rm R}\left(4\varepsilon^2+\Gamma_{\rm R}^2\right) \\ & + (\gamma_1+\gamma_2)\left[4\Gamma_{\rm L}\left(\varepsilon^2+2\Omega^2\right) + 4\Omega^2\Gamma_{\rm R}\right. \\ & + \Gamma_{\rm L}(\gamma_1+\gamma_2)^2 + \Gamma_{\rm R}(\gamma_2+3\Gamma_{\rm L})(\gamma_1+\gamma_2) \\ & \left. + \Gamma_{\rm R}^2(2\gamma_2+3\Gamma_{\rm L})\right],\end{aligned} \tag{35a}$$

$$\begin{aligned}\Xi = {} & \lambda_2\left(\Gamma_{\rm L}+\alpha^2\Gamma_{\rm R}\right) + \lambda_1\left(\Gamma_{\rm L}+\beta^2\Gamma_{\rm R}\right) \\ & + \Gamma_{\rm R}\left[\left(\alpha^4+\beta^4\right)\Gamma_{\rm L} + \alpha^2\beta^2\Gamma_{\rm R}\right].\end{aligned} \tag{35b}$$

Figure 2 shows the calculated values $I_{\rm o}^{\rm s}$ and $I_{\rm e}^{\rm s}$ of the stationary current through the DQD. We choose a typical interdot coupling $\Omega = 32$ μeV, which is experimentally accessible.[39] For both $I_{\rm o}^{\rm s}$ and $I_{\rm e}^{\rm s}$ at the resonant tunneling point characterized by $\varepsilon_1 - \varepsilon_2 = 0$, the current reaches its maximum. Moreover, it can be seen that the current is asymmetric around the maximum point. This asymmetry was also observed in a recent experiment by Barthold *et al.*[7] It is due to dissipations induced by the phonon bath, as we will now demonstrate. In the absence of electron–phonon coupling, we have $\gamma_1 = \gamma_2 = 0$ and $\lambda_1 = \lambda_2 = 0$, so that Eqs. (34a) and (34b) reduces to

$$I_{\rm o}^{\rm s} = \frac{e4\Omega^2\Gamma_{\rm L}\Gamma_{\rm R}}{4\Omega^2(2\Gamma_{\rm L}+\Gamma_{\rm R}) + 4\varepsilon^2\Gamma_{\rm L} + \Gamma_{\rm L}\Gamma_{\rm R}^2}, \tag{36a}$$

$$I_{\rm e}^{\rm s} = \frac{e4\Omega^2\Gamma_{\rm L}\Gamma_{\rm R}}{4\Omega^2(2\Gamma_{\rm L}+\Gamma_{\rm R}) + 4\varepsilon^2\Gamma_{\rm L}}, \tag{36b}$$

where Eq. (37a) agrees with the result from previous studies,[8,40] in which the occupation-state basis was also used. From Eqs. (37a) and (37b), it is clear that the current as predicted using either the occupation-state basis or the eigenstate basis is symmetric about the current peak at $\varepsilon_1 = \varepsilon_2$. This reveals that this asymmetry of the current is due to the coupling of the DQD to the phonon bath.

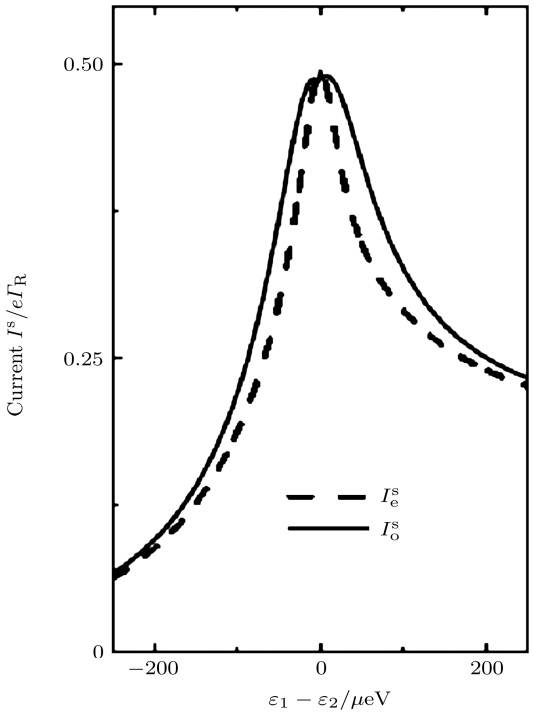


Fig. 2. Stationary current $I^{\rm s}$ through the DQD as a function of the energy difference $\varepsilon_1 - \varepsilon_2$ calculated using the occupation-state basis ($I^{\rm s} = I_{\rm o}^{\rm s}$) and the eigenstate basis ($I^{\rm s} = I_{\rm e}^{\rm s}$) for a large interdot coupling $\Omega = 32$ μeV. We have taken $\Gamma_{\rm L} = 100$ μeV, $\Gamma_{\rm R} = 2.5$ μeV, $\gamma_0 = 0.6$ μeV, and $T = 2$ K.

As shown in Section 2, the master equation derived in the occupation-state basis is only valid in the limit of a weak interdot coupling, i.e., $\Omega \ll |\varepsilon_2 - \varepsilon_1|$ while that in the eigenstate basis is valid for any arbitrary interdot coupling. Figure 3 plots the values of the stationary current calculated in the two bases for a small interdot coupling ($\Omega = 1$ μeV). As expected, when the interdot coupling Ω is much smaller than the energy difference $|\varepsilon_2 - \varepsilon_1|$ of the two dots, the stationary-state current calculated in the occupation-state basis agrees very well with that in the eigenstate basis, as is evident from Fig. 3. However, when the interdot coupling is comparable to the energy difference, the stationary currents in the occupation-state basis deviates drastically from the stationary current in the eigenstate basis (see Fig. 2). This deviation can also be revealed in Fig. 3 in the narrow region with $|\varepsilon_2 - \varepsilon_1| \sim \Omega$ ($= 1$ μeV) (see the inset of Fig. 3). These clearly show the inaccuracy of the current and hence the master equation in the occupation-state basis at large Ω. In this case, one must use the master equation derived in the eigenstate basis.

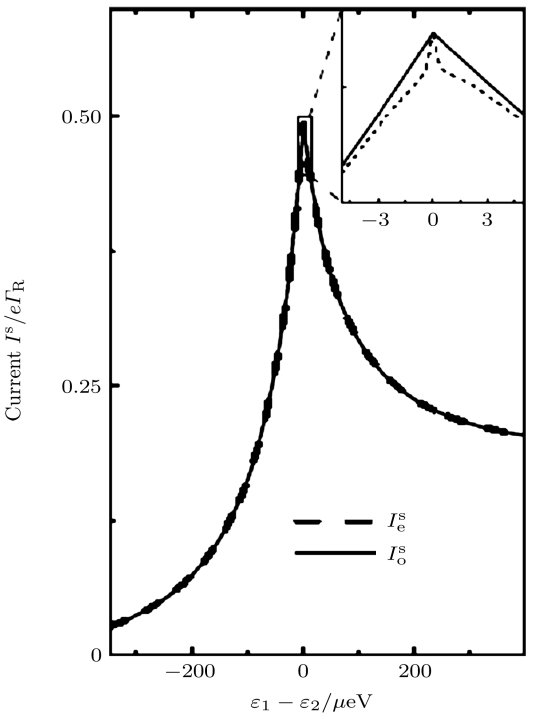


Fig. 3. Stationary current $I^{\rm s}$ as a function of $\varepsilon_1 - \varepsilon_2$ calculated using the occupation-state basis ($I^{\rm s} = I^{\rm s}_{\rm o}$) and the eigenstate basis ($I^{\rm s} = I^{\rm s}_{\rm e}$) for a small interdot coupling $\Omega = 1$ μeV. Inset: The enlarged diagram of the stationary current $I^{\rm s}$ in the region with $\varepsilon_1 - \varepsilon_2$ comparable to Ω. All the parameters except the interdot coupling are the same as those used in Fig. 2.

4. Shot noise

Following the previous studies,[16,19,41] one can calculate the Fano factor that characterises the shot noise in the tunneling current through the DQD. We first consider the results based on the occupation-state basis. Using the master equation (24), the Fano factor $F_{\rm o}$ in the occupation-state basis is found to be

$$F_{\rm o} = 1 + 2 \times \frac{a_1 a_4 - a_2 a_3}{a_2^2}, \tag{37}$$

where

$$\begin{aligned} a_1 =& -\frac{1}{4}\Gamma_{\rm L}\Gamma_{\rm R}\left\{4\varepsilon^2\gamma_2 + (\gamma_1+\gamma_2+\Gamma_{\rm R})\right. \\ & \left. \times \left[4\Omega^2 + \gamma_2\left(\gamma_1+\gamma_2+\Gamma_{\rm R}\right)\right]\right\}, \end{aligned}$$

$$\begin{aligned} a_2 =& \frac{1}{4}\left\{\begin{array}{l} \Gamma_{\rm L}\left(\gamma_1+\gamma_2\right)\left[4\left(\varepsilon^2+2\Omega^2\right)+\left(\gamma_1+\gamma_2\right)^2\right] \\ +\left[\left(\gamma_1+\gamma_2\right)\left(4\Omega^2+\gamma_2\left(\gamma_1+\gamma_2\right)\right)+\left(8\Omega^2+3\left(\gamma_1+\gamma_2\right)^2\right)\Gamma_{\rm L}+4\varepsilon^2\left(\gamma_2+\Gamma_{\rm L}\right)\right]\Gamma_{\rm R} \\ +\left[4\Omega^2+\left(\gamma_1+\gamma_2\right)\left(2\gamma_2+3\Gamma_{\rm L}\right)\right]\Gamma_{\rm R}^2+\left(\gamma_2+\Gamma_{\rm L}\right)\Gamma_{\rm R}^3 \end{array}\right\}, \\ a_3 =& -\Gamma_{\rm L}\Gamma_{\rm R}\left[2\Omega^2+\gamma_2\left(\gamma_1+\gamma_2+\Gamma_{\rm R}\right)\right], \\ a_4 =& \frac{1}{4}\left\{\begin{array}{l} \gamma_1^3+\gamma_2^3+4\left(\varepsilon^2+4\Omega^2\right)\left(\Gamma_{\rm L}+\Gamma_{\rm R}\right)+5\Gamma_{\rm L}\Gamma_{\rm R}^2+\Gamma_{\rm R}^3+\gamma_1^2\left(3\gamma_2+5\Gamma_{\rm L}+3\Gamma_{\rm R}\right) \\ +\gamma_2^2\left(5\Gamma_{\rm L}+7\Gamma_{\rm R}\right)+\gamma_2\left(4\varepsilon^2+8\Omega^2+10\Gamma_{\rm L}\Gamma_{\rm R}+7\Gamma_{\rm R}^2\right) \\ +\gamma_1\left(4\varepsilon^2+8\Omega^2+3\gamma_2^2+10\Gamma_{\rm L}\Gamma_{\rm R}+3\Gamma_{\rm R}^2+10\gamma_2\left(\Gamma_{\rm L}+\Gamma_{\rm R}\right)\right) \end{array}\right\}. \end{aligned} \tag{38}$$

Alternatively, using the eigenstate basis, one can obtain from Eq. (31) that the Fano factor $F_{\rm e}$ in the eigenstate basis is given by

$$F_{\rm e} = 1 + \frac{2\Gamma_{\rm L}\Gamma_{\rm R}}{\Xi^2} \times \left\{2\alpha^2\beta^2\Xi - \left(\lambda_1+\lambda_2+\Gamma_{\rm L}+\Gamma_{\rm R}\right) \times \left[\beta^2\lambda_1+\alpha^2\lambda_2+\alpha^2\beta^2\Gamma_{\rm R}\right]\right\}, \tag{39}$$

where

$$b_1 = -\Gamma_{\rm L}\Gamma_{\rm R}\left[\alpha^2\left[\lambda_2+\beta^2\Gamma_{\rm R}\right]+\beta^2\lambda_1\right],$$

$$b_2 = \lambda_1 \left[\Gamma_{\rm L} + \Gamma_{\rm R}\beta^2\right] + \lambda_2 \left[\Gamma_{\rm L} + \Gamma_{\rm R}\alpha^2\right] + \Gamma_{\rm R} \left[\Gamma_{\rm L} \left(1 - 2\alpha^2\beta^2\right) + \alpha^2\beta^2\Gamma_{\rm R}\right],$$
$$b_3 = -2\alpha^2\beta^2\Gamma_{\rm L}\Gamma_{\rm R},$$
$$b_4 = \lambda_1 + \lambda_2 + \Gamma_{\rm L} + \Gamma_{\rm R}. \tag{40}$$

Without any phonon dissipation effect, i.e., $\gamma_1 = \gamma_2 = 0$ or $\lambda_1 = \lambda_2 = 0$, the Fano factors become

$$F_{\rm o} = 1 - \frac{8\Omega^2\Gamma_{\rm L}\left[4\varepsilon^2\left(\Gamma_{\rm R} - \Gamma_{\rm L}\right) + 3\Gamma_{\rm L}\Gamma_{\rm R}^2 + \Gamma_{\rm R}^3 + 8\Omega^2\Gamma_{\rm R}\right]}{\left[\Gamma_{\rm L}\Gamma_{\rm R}^2 + 4\Gamma_{\rm L}\varepsilon^2 + 4\Omega^2\left(\Gamma_{\rm R} + 2\Gamma_{\rm L}\right)\right]^2}, \tag{41}$$

$$F_{\rm e} = 1 - \frac{8\Omega^2\Gamma_{\rm L} \times \left\{4\varepsilon^2\left(\Gamma_{\rm R} - \Gamma_{\rm L}\right) + 8\Omega^2\Gamma_{\rm R}\right\}}{\left[4\varepsilon^2\Gamma_{\rm L} + 4\Omega^2\left(2\Gamma_{\rm L} + \Gamma_{\rm R}\right)\right]^2}. \tag{42}$$

Here $F_{\rm o}$ is identical to the previous results[40,41] obtained in the occupation-state basis. For a super-Poissonian noise, one has $F_{\rm o} > 1$. It is obtained from Eq. (42) when the following condition is needed

$$4\varepsilon^2\left(\Gamma_{\rm L} - \Gamma_{\rm R}\right) > 3\Gamma_{\rm L}\Gamma_{\rm R}^2 + \Gamma_{\rm R}^3 + 8\Omega^2\Gamma_{\rm R}. \tag{43}$$

Figure 4 presents both of the calculated Fano factors $F_{\rm o}$ and $F_{\rm e}$ of the shot noise based on the occupation-state basis and eigenstate basis, respectively. At the resonant tunneling point, i.e., $\varepsilon_2 = \varepsilon_1$, both approaches predict that the shot noise is sub-Poissonian. For $F_{\rm o}$, in the absence of phonon-induced dissipation, a super-Poissonian noise can be obtained in the condition Eq. (43). Due to the effects of dissipation, $F_{\rm o}$ has only sub-Poissonian noise for the whole parameter range investigated here. In contrast, $F_{\rm e}$ has much richer behaviours of super-Poissonian, sub-Poissonian, and Poissonian noise correlations, depending on the energy difference $\varepsilon_1 - \varepsilon_2$. Moreover, $F_{\rm e}$, but not $F_{\rm o}$, exhibits a double-peak structure and an asymmetry around the dip at $\varepsilon_2 = \varepsilon_1$. These features were also observed in a recent experiment.[7]

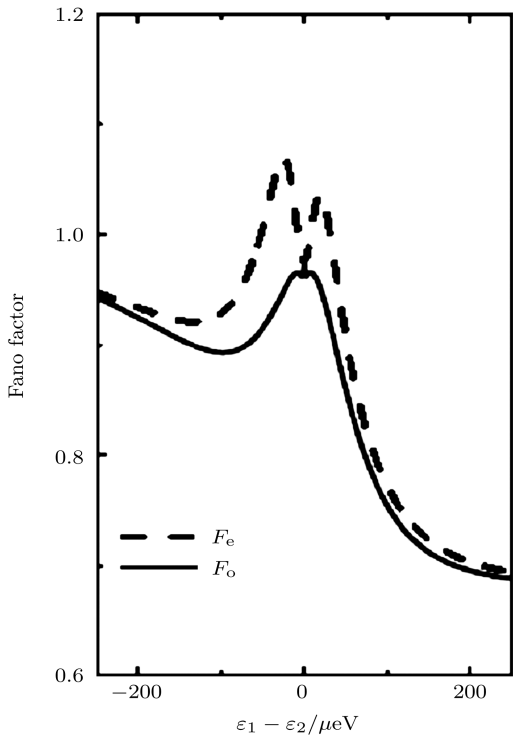


Fig. 4. Fano factor F as a function of $\varepsilon_1 - \varepsilon_2$ calculated using the occupation-state basis ($F = F_{\rm o}$) and the eigenstate basis ($F = F_{\rm e}$) for a large interdot coupling $\Omega = 32$ μeV. All the other parameters are the same as those in Fig. 2.

Certain characteristic features found in experiments have been successfully reproduced using the occupation-state basis.[8] Nevertheless, previous calculations threw little insight on the physical origin of the double peak in the Fano factor observed. Now, it can be intuitively understood using the eigenstate basis as follows. The electrons can tunnel from the DQD to the right lead via two channels, namely, the ground-state channel and the excited-state channel. The effective tunneling rates are defined as

$$\Gamma_{\rm g} \equiv \Gamma_{\rm R}\beta^2 = \Gamma_{\rm R}\frac{\Omega_0 - \varepsilon}{2\Omega_0},$$
$$\Gamma_{\rm e} \equiv \Gamma_{\rm R}\alpha^2 = \Gamma_{\rm R}\frac{\Omega_0 + \varepsilon}{2\Omega_0}. \tag{44}$$

At the resonant tunneling point ($\varepsilon_2 = \varepsilon_1$), the tunnel rate through the ground-state channel is the same as that through the excited-state channel. This results in a sub-Poissonian shot noise.[15] When $\varepsilon_2 > \varepsilon_1$, one has $\Gamma_{\rm g} < \Gamma_{\rm e}$, and the electron transport through the ground-state channel blocks that through the excited-state channel. This dynamical channel blockade leads to a super-Possionian shot noise.[15]

However, when $\varepsilon_2 - \varepsilon_1 \gg \Omega$, $\Gamma_{\rm g}$ becomes zero and the electron can only tunnel through the DQD via the excited-state channel. This single-channel tunneling gives rise to a sub-Poissonian shot noise,[13] as shown in Fig. 4. Similarly, when $\varepsilon_2 < \varepsilon_1$, one has $\Gamma_{\rm g} > \Gamma_{\rm e}$ and the tunneling through the excited-state channel blocks that through the ground-state channel.

The noise is super-Poissonian for a small energy difference $|\varepsilon_2 - \varepsilon_1|$, due to the dynamical channel blockade. When $\varepsilon_1 - \varepsilon_2 \gg \Omega$, $\Gamma_{\rm e}$ becomes zero and the electron can only tunnel through the DQD via the ground-state channel. This single-channel tunneling also gives rise to a sub-Poissonian noise. The asymmetry of the Fano factor is caused by the relaxation process induced by the electron–phonon interaction. When $\varepsilon_2 > \varepsilon_1$, we have $\Gamma_{\rm g} < \Gamma_{\rm e}$ and the relaxation process from the excited state to the ground state enhances the dynamical channel blockade. However, when $\varepsilon_2 < \varepsilon_1$, one has $\Gamma_{\rm g} > \Gamma_{\rm e}$ and the relaxation process from the excited state to the ground state suppresses the dynamical channel blockade. The asymmetry of the Fano factor hence follows [see Fig. 4].

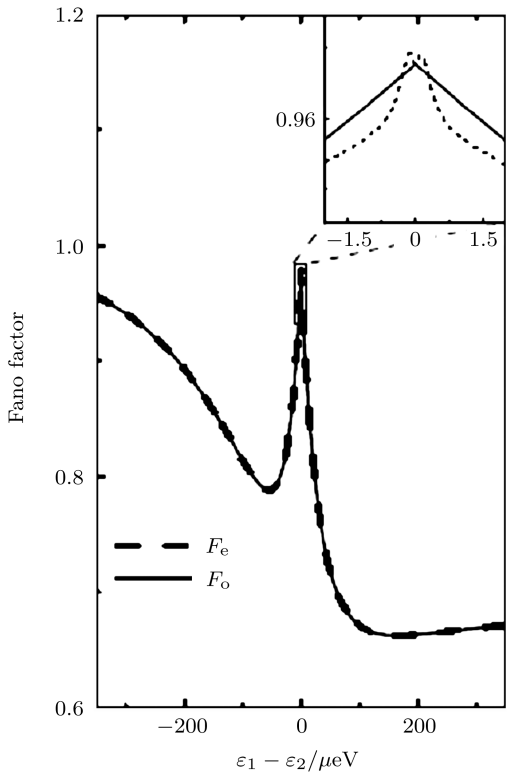


Fig. 5. Fano factor F as a function of $\varepsilon_1 - \varepsilon_2$ calculated using the occupation-state basis ($F = F_{\rm o}$) and the eigenstate basis ($F = F_{\rm e}$) for a small interdot coupling $\Omega = 1$ μeV. All the other parameters are the same as those in Fig. 2. Inset: The enlarged diagram of the Fano factor F in the region with $|\varepsilon_2 - \varepsilon_1|$ comparable to Ω.

We have shown using Fig. 4 that for a large interdot coupling, e.g., $\Omega = 32$ μeV, the Fano factor in the occupation-state basis deviates drastically from the Fano factor in the eigenstate basis. This verifies that the small interdot coupling approximation in deriving the master equation in the occupation-state basis is invalid. Instead, the master equation in the eigenstate basis should be used. As a further consistency check, Figure 5 shows the Fano factor of the shot noise for a small interdot coupling strength ($\Omega = 1$ μeV). As expected, the calculated Fano factors using both basis agrees with each other except for the small region with $|\varepsilon_2 - \varepsilon_1| \sim \Omega$; in this small region, the results in the two cases are different because the condition $|\varepsilon_2 - \varepsilon_1| \gg \Omega$ is not satisfied (see the inset of Fig. 5).

5. Conclusions

In summary, we have derived two master equations in both the occupation-state basis and the eigenstate basis to describe the dynamics of the DQD. We show that the master equation in the occupation-state basis is only valid for a small interdot coupling, while the master equation in the eigenstate basis is valid for an arbitrary interdot coupling. To demonstrate the difference between these two master equations, we focus on the current and shot-noise properties in electron tunneling through the DQD. When the interdot coupling is much smaller than the energy difference between the two dots, the current and shot noise in the occupation-state basis are very close to those in the eigenstate basis. For a large interdot coupling, however, the properties derived in the occupation-state basis deviate drastically from those in the eigenstate basis. This reveals that the master equation in the occupation-state basis is not accurate for the case of a large interdot coupling and in this case the master equation in the eigenstate basis should be used. Also, we show that the shot-noise properties predicted using the eigenstate basis can successfully reproduce the features found in a recent experiment.[7]

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